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THOMAS-FERMI EQUATION OF STATE–THE HOT CURVE

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ABSTRACT

We derive the high-temperature limit of the equation of state based on the Thomas-Fermi statistical theory of the atom. The resulting "hot curve" is in fact the ideal Fermi gas. We expand the thermodynamic properties of this gas in powers of the fugacity and use this expansion to construct a representation of the pressure, accurate to about 0.1 %. This representation is compared with the actual theory for aluminum and the "hot curve" is found to represent it well over a large region of interest in applications.

1. INTRODUCTION AND SUMMARY

The Thomas-Fermi (T-F) statistical theory of the atom[1] as well as the modifications due to Dirac[2] have long been used as a basic starting point for the computation of approximations to the equations of state.[3,4] In order to make use of this procedure, computer programs have been written to compute the numerical content of the theory. They consume a sufficient amount of computer time, even today, so that it is impractical to use them to compute, *ab initio*, the value of the pressure, internal energy, *etc.*, every time that a new value is required inside an application computer program. Besides, as these efforts represent only approximate equations of state, some adjustment is necessary to bring them into accord with physical reality. Consequentially, to date largely empirical fits have been used to represent the equations of state for the purposes of applications.

In this work, we are concerned with beginning an analysis of the physical structure of the equations of state of real matter. As a start, we will study the Thomas-Fermi model equation of state which represents a fair amount of the physics, at least in some regions. One method which is normally fruitful, is to consider various limits. There are currently two which are known. The first is the low-density limit. Here there is complete ionization when the system is in equilibrium and the pressure for an element of nuclear charge Z is

$$P\Omega/N = (Z+1)kT, \tag{1.1}$$

the ideal gas equation of state. Here P is the pressure, Ω is the volume of the system, N is the number of atoms, k is Boltzmann's constant and T is the absolute temperature. The second limit[3] is the low-temperature limit, or the "cold curve." Here the pressure is of the form,

$$P\Omega/N = Z^{\frac{7}{3}}\phi(Z\Omega/N), \tag{1.2}$$

where $\phi(x)$ is a well defined function. If we think of the temperature-density, quarter-plane, these results give the limiting behavior of the T-F model along the zero-temperature and the zero-density edges. There remain the high-density and the high-temperature regions to examine for physical structure.

One might think that in the high-temperature limit it would be appropriate to describe the system in purely classical terms. Indeed if such were the case, Baker[5] has proven that the pressure would be of the form,

$$P\Omega/N = kT\, f(\Omega T^3/N, Z). \tag{1.3}$$

The Debye-Hückel correction[6] is of just this form. Also Baker has shown for this case that the internal energy has the particularly simple form,

$$u = 3P\Omega - \frac{3}{2}(Z+1)NkT. \tag{1.4}$$

The statistical mechanics of Coulombic systems have been much studied.[7] It is now well known that there does not exist a classical (*i.e.* Planck's constant $h = 0$) gas because atoms with a Coulomb interaction collapse to $E = -\infty$. Thus if we are to ever introduce a Coulomb attraction between the atomic nucleus and the electrons, we must necessarily include some account of the quantum effects that are needed to stabilize the system. As is also well known there are two important physical lengths to be considered. The first is the de Broglie length which is proportional to $h/\sqrt{mkT}$, where m is the electron mass, and which measures in a noninteracting gas the importance of quantum effects. The Coulomb interaction does not by itself provide the second length and the difficulty of its long range can not be circumvented by studying dilute systems because it contains no parameter with the dimensions of

a length. The second length is the Debye screening length which is proportional to e^2/kT. This length is however a statistical effect and should follow from the theory, but unfortunately is not there *ab initio*. Thus when we look to the high-temperature and high-density regions, if we consider the cases where $\Omega/N >> (e^2/kT)^3$, then we can hope to start with a noninteracting electron gas (with a background gas of atomic nuclei) as the basic system.

In the second section, we derive the limit of Thomas-Fermi theory when the Debye screening length is negligible compared to the interparticle distance, and the de Broglie length remains arbitrary. We find that it correctly reduces to the ideal Fermi gas. We call this limit the "hot curve," because it is reached if one either fixes the density and lets the temperature go to infinity, or much less restrictively, it is also reached if one fixes the de Broglie length and then lets the temperature go to infinity. In the third section we review the theory of the ideal Fermi gas and describe how to calculate its properties in a practical manner. We derive lengthy fugacity series and find that the pressure function can be approximated to within, say 0.1%, by a low-order, two-point Padé approximant. In the final section we compare the ideal gas approximation to results for aluminum and map out its region of validity to various degrees of accuracy.

2. HIGH TEMPERATURE LIMIT OF THOMAS–FERMI THEORY

Thomas-Fermi theory has been applied to compute equations of state at finite temperature by Feynman *et al.*[3] They begin with an application of the statistical analysis of Fermi and Dirac which leads to the equation

$$\rho = \int_0^\infty \frac{2 \cdot 4\pi p^2\, dp/h^3}{\exp[(p^2/2m - eV)/kT + \eta] + 1}, \tag{2.1}$$

where $-eV$ is the potential energy. We follow them in defining for convenience the auxiliary functions

$$I_n(\eta) = \int_0^\infty \frac{y^n dy}{\exp(y - \eta) + 1}. \tag{2.2}$$

Then one uses Poisson's equation to determine V(r). It yields

$$\frac{1}{r}\frac{d^2}{dr^2}(rV(r)) = \frac{16\pi^2}{h^3}e(2mkT)^{\frac{3}{2}}I_{\frac{1}{2}}\left(\frac{eV(r)}{kT} - \eta\right). \tag{2.3}$$

Note that in the case of no interaction that the right-hand side of (2.3) vanishes (e=0) and so the equation implies that $V = a + b/r$ where a and b are constants. In order to simplify the above equation, Feynman *et al.*[3] introduce dimensionless variables. First they define a length scale,

$$c = \left(\frac{h^3}{32\pi^2 e^2 m(2mkT)^{\frac{1}{2}}}\right)^{\frac{1}{2}} \propto T^{-\frac{1}{4}}, \tag{2.4}$$

where $s = r/c$. Then since η is independent of r, (2.3) becomes

$$\frac{d^2\beta}{ds^2} = sI_{\frac{1}{2}}(\beta/s), \tag{2.5}$$

where

$$\beta/s = (eV(r)/kT) - \eta. \tag{2.6}$$

The boundary conditions of (2.5) become, as at the origin $V(r)$ must behave as Ze/r,

$$\beta(0) = \alpha = Ze^2/kTc \propto T^{-\frac{3}{4}}. \tag{2.7}$$

The scheme employed is to suppose that each atom is confined to a sphere of volume equal to the volume per particle. This is clearly an approximation. The other boundary condition is to require that the number of electrons in the sphere is exactly equal to the nuclear charge. A little manipulation serves to show that the condition,

$$\frac{d\beta}{ds} = \beta/s \text{ at } s = b, \tag{2.8}$$

imposes this normalization in the sphere of radius $r = cb$. Feynman *et al.*[3] derive, among other things, the formula for the pressure as

$$P\Omega/N = \frac{2}{9}(ZkT) \cdot \frac{b^3}{\alpha} I_{\frac{3}{2}}\left(\frac{\beta_b}{b}\right), \tag{2.9}$$

where β_b is the value of β on the boundary $s = b$.

In a parallel way we may set out the corresponding formulae for the ideal Fermi gas. In this case the electron density is simply given by (2.1) with $e = 0$. As η is independent of r, one sees immediately by (2.6) that the equation for the density (2.5) is simply satisfied. Since by (2.4) and (2.7) both the length and magnitude scales depend on the electronic charge $e = 0$, the normalization equation (2.8), in leading order, is automatically satisfied, and so does not determine the number of electrons in this limit. Returning to (2.1), we may impose the normalization condition by integrating the density over a sphere of radius r. It gives

$$Z = \frac{16\pi^2}{3} I_{\frac{1}{2}}(-\eta) \left[\frac{r\sqrt{2mkT}}{h}\right]^3, \tag{2.10}$$

which implies η. In this limit, the pressure equation (2.9), becomes,

$$P\Omega/N = \frac{2}{9}(ZkT)\left(\frac{r^3}{c^3\alpha}\right) I_{\frac{3}{2}}(-\eta), \tag{2.11}$$

a parametric expression for the pressure in terms of the η of (2.10). Note is made that $c^3\alpha$ is independent of the electronic charge $e = 0$, so this form is valid in this noninteracting limit. Comparison with the results of Huang[8] for the ideal Fermi gas, reveal complete agreement, when it is remembered that for our case the spin, $s = \frac{1}{2}$.

Now we are ready to consider the "hot curve" limit of the Thomas-Fermi theory. In the basic equations of the theory, (2.5, 7-8), we make the following change of variables,

$$\sigma = s/\alpha^{\frac{1}{3}}, \ \gamma = \beta/\alpha^{\frac{1}{3}}. \tag{2.12}$$

We thus obtain

$$\frac{d^2\gamma}{d\sigma^2} = \alpha^{\frac{2}{3}}\sigma I_{\frac{1}{2}}\left(\frac{\gamma}{\sigma}\right), \tag{2.13}$$

$$\gamma(0) = \alpha^{\frac{2}{3}}, \tag{2.14}$$

$$\frac{d\gamma}{d\sigma} = \frac{\gamma}{\sigma}, \text{ at the boundary.} \tag{2.15}$$

In the limit $\alpha \to 0$ (by (2.7) this limit is equivalent to $T \to \infty$), we obtain the result that $\gamma = A\sigma$ solves (2.13-15). Again, as at (2.10) above, we have an undetermined normalization constant to be determined because in our high-temperature limit (2.15) is satisfied automatically. Again referring to (2.1) we obtain the normalization condition,

$$Z = \frac{16\pi^2}{3h^3}[r\sqrt{2mkT}]^3 I_{\frac{1}{2}}\left(\frac{\gamma}{\sigma}\right),\tag{2.16}$$

which determines A and thus the solution of (2.13-15). When we note the comparison $A = -\eta$, we find that this limiting solution is the same as the one we obtained for the ideal (noninteracting) Fermi gas. This result completes our demonstration of the proposition that the "hot curve" for Thomas-Fermi theory is the ideal Fermi gas!

3. PROPERTIES OF THE IDEAL FERMI GAS

The basic theory of the ideal Fermi gas is described by Huang.[8] To establish a correspondence between the results of the previous section and more standard notation, we note that in (2.16) $\gamma/\sigma = A$; therefore we introduce the notation $z = e^{-A}$. We can then rewrite (2.16) and (2.11) as

$$\frac{ZN}{\Omega} = \frac{3Z}{4\pi r^3} = 2\left(\frac{2\pi mkT}{h^2}\right)^{\frac{3}{2}} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{zy^{\frac{1}{2}}e^{-y}dy}{1 + ze^{-y}},\tag{3.1}$$

$$\frac{P}{kT} = 2\left(\frac{2\pi mkT}{h^2}\right)^{\frac{3}{2}} \frac{4}{3\sqrt{\pi}} \int_0^\infty \frac{zy^{\frac{3}{2}}e^{-y}dy}{1 + ze^{-y}},\tag{3.2}$$

where P is the pressure due to the electrons only and does not take account of the effect of the motion of the center of mass of the atom. If we introduce the further notation,

$$\lambda = \left(\frac{h^2}{2\pi mkT}\right)^{\frac{1}{2}},\tag{3.3}$$

$$f_{\frac{3}{2}}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{zy^{\frac{1}{2}}e^{-y}dy}{1 + ze^{-y}} = \sum_{l=1}^\infty \frac{(-1)^{l+1}z^l}{l^{\frac{3}{2}}},\tag{3.4}$$

$$f_{\frac{5}{2}}(z) = \frac{4}{3\sqrt{\pi}} \int_0^\infty \frac{zy^{\frac{3}{2}}e^{-y}dy}{1 + ze^{-y}} = \sum_{l=1}^\infty \frac{(-1)^{l+1}z^l}{l^{\frac{5}{2}}},\tag{3.5}$$

where the series expansions are convergent for $|z| \le 1$. We may now rewrite (3.1-2) as

$$\zeta = \frac{ZN\lambda^3}{2\Omega} = f_{\frac{3}{2}}(z),\tag{3.6}$$

and

$$\frac{P\Omega}{ZNkT} = \frac{f_{\frac{5}{2}}(z)}{f_{\frac{3}{2}}(z)},\tag{3.7}$$

where ζ is the de Broglie density. The procedure to calculate the pressure of the ideal Fermi gas is now, in principle, quite straightforward. Eq. (3.6) is solved for z and then that value is substituted into (3.7).

To evaluate these expressions numerically we choose the following method. First we revert the series expansion (3.6) to give $z(\zeta)$ as a series in ζ. Then we substitute it into (3.7) to obtain

$$\frac{P\Omega}{ZNkT} = g(\zeta).\tag{3.8}$$

We have calculated the leading 36 terms of the series expansion. The method used is the classical Lagrange formula for the reversion of series.[9] The only point of difficulty is that a large number of decimal places are lost in the computation in this case. We have therefore taken the precaution of using at least 58 decimal places to carry out these computations. The results are listed in Table 1.

TABLE 1. $(P\Omega/ZNkT)$ as a series in the de Broglie density

0	1.0000000000 0000000000 0000000000 0000000000 00000000000000000E+000
1	1.7677669529 6636881100 2110905262 1225982120 8984422118509147E-001
2	-3.3000598199 1683655758 8617889323 8790328003 89171139305782E-003
3	1.1128932846 6542504524 9253533917 1305775999 1875768224181E-004
4	-3.5405040951 9736538278 3050093233 4626176046 46439677965E-006
5	8.3863470395 6925729619 7125848681 6218474298 427436245E-008
6	-3.6620617873 4852703663 1688233937 9045907824 8643167E-010
7	-1.0280607154 3957929799 3273512206 9735581999 5254513E-010
8	7.0550978435 7263454626 0275709452 8261969773 09158E-012
9	-2.6859639507 9285424406 0526716388 7926863588 4377E-013
10	4.0571834908 0612166197 1056127182 3091151601 35E-015
11	2.7970439770 9162019148 3071234746 1358106846 6E-016
12	-2.8379673439 5952590529 6631787032 9726025304 E-017
13	1.3992940717 5922219970 7552151122 203412696E -018
14	-3.6303052861 0821033013 0082398676 2418074E-0 20
15	-6.0257400821 7251347692 8112664253 67093E-022
16	1.2989538153 2549763684 7035089386 73544E-022
17	-8.1719971340 6344259697 7319803759 795E-024
18	2.9413082494 4946667164 3606073469 73E-025
19	-2.0285711098 2088612486 4658243931 E-027
20	-5.7410636166 7615749309 984730023E -028
21	4.8461575378 3763503589 33968480E- 029
22	-2.2369786852 5871386652 1846940E-0 30
23	4.7888680538 7474310454 78772E-032
24	2.0304880286 8391265410 8553E-033
25	-2.7811009124 7360566430 414E-034
26	1.6149810555 1163427972 12E-035
27	-5.2554355032 5730228297 E-037
28	-1.3309033541 33284697E- 039
29	1.4721238409 86015824E- 039
30	-1.1062516681 9956070E-0 40
31	4.7267873838 86169E-042
32	-7.6386716803 536E-044
33	-6.5324794996 62E-045
34	7.1193401844 5E-046
35	-3.8268661579 E-047
36	1.097950074E -048

The above series expansion was derived for $|z| \le 1$, but the above series plainly corresponds to a larger range. In the limit as $z \to \infty$ Huang shows that

$$f_{\frac{3}{2}}(z) \asymp \frac{4}{3\sqrt{\pi}}(\log z)^{\frac{3}{2}} \left[1 + \frac{\pi^2}{8(\log z)^2} + \cdots\right] + O(z^{-1}). \qquad (3.9)$$

From the identity,[8] $z\frac{d}{dz}f_{\frac{5}{2}}(z) = f_{\frac{3}{2}}(z)$ one can easily also derive the asymptotic behavior of $f_{\frac{5}{2}}(z)$, and thus from (3.7) the asymptotic behavior of $g(\zeta)$. We obtain,

$$g(\zeta) \asymp \frac{2}{5}\left(\frac{3\sqrt{\pi}}{4}\right)^{\frac{2}{3}} \zeta^{\frac{2}{3}} \text{ as } \zeta \to \infty. \qquad (3.10)$$

With this information and the series of Table 1, we may construct a two point Padé approximant[10] to $[g(\zeta)]^3$ of the form $[N + 2/N]$ which is exact through order ζ^{2N+1} at the origin, and is also asymptotically correct as $\zeta \to \infty$. We find excellent convergence for this method and that for $0 \leq \zeta < \infty$ we get an accuracy of about 0.1 percent for $g(\zeta)$ from the approximation,

$$g(\zeta) \approx \left[\frac{1 + 0.61094880\zeta + 0.12660436\zeta^2 + 0.0091177644\zeta^3}{1 + 0.080618739\zeta} \right]^{\frac{1}{3}}. \tag{3.11}$$

Thus the total pressure would be (including the center of mass motion)

$$P = \frac{NkT}{\Omega}\{1 + Zg(\zeta)\}. \tag{3.12}$$

In the case where the temperature is fixed and $\Omega \to \infty$, the low-density limit, not only does the Debye density go to zero, as required to obtain the ideal Fermi gas limit of Thomas-Fermi theory, but also $\zeta \to 0$. In this case, as $g(0) = 1$, (3.12) reduces to (1.1) and thereby supplies an alternate derivation of the low-density limit of Thomas-Fermi theory.

As Huang[8] points out, the internal energy, U, for this case follows simply from (3.12) as,

$$U = \frac{3}{2}P\Omega. \tag{3.13}$$

Epstein[11] shows from the thermodynamic relation $dS = (dU + PdV)/T$, the above results, and Nernst's heat postulate that the entropy of the ideal Fermi gas is simply given by

$$S_e = ZNk\left(\frac{5}{2}g(\zeta) - \log z(\zeta)\right), \tag{3.14}$$

where the limit as $T \to 0$ is the limit $\zeta \to \infty$ by (3.6) and as Epstein further points out $S_e \to 0$ in this limit. If we add the contribution of the motion of the center of mass to the entropy, we get

$$S = Nk\left[-(Z+1)\log\zeta + \frac{5}{2} + Z\left(\frac{5}{2}g(\zeta) - \log[z(\zeta)/\zeta]\right)\right] + \text{constant}, \tag{3.15}$$

The Helmholtz free energy is now given directly by $A = U - TS$. The Gibbs thermodynamic potential is also directly given and is $G = U - TS + P\Omega$.

It now remains to give a representation of $\log z(\zeta) = \log \zeta + \log[z(\zeta)/\zeta]$ to complete the representation of the thermodynamic quantities for the ideal Fermi gas. Since $\log z \asymp \zeta^{\frac{2}{3}}$, the problem of deriving a representation for $\log[z(\zeta)/\zeta]$ should be similar to that of the representation (3.11). We give in Table 2 the necessary series coefficients in ζ for $z(\zeta)$ to work on this representation, but we will leave it for the future. Thermodynamic consistency depends on the equation between the two representations

$$g(\zeta) + \zeta g'(\zeta) = \zeta \frac{d \log z(\zeta)}{d\zeta}. \tag{3.16}$$

TABLE 2. The fugacity z as a series in the de Broglie density

1	1.0000000000 0000000000 0000000000 0000000000 00000000000000000E+000
2	3.5355339059 3273762200 4221810524 2451964241 7968844237018294E-001
3	5.7549910270 1247451636 1707316601 4181450799 416243291041327E-002
4	5.7639604009 1025440341 8852781947 0758923518 58214221729707E-003
5	4.0194941515 2300959555 6172119656 7773364832 0998466829345E-004
6	2.0981898872 2604799054 4860297423 5099614729 957102872728E-005
7	8.6021310842 6030566004 3913343164 3181688359 0277772573E-007
8	2.8647148623 7664872936 8242210245 0573640824 266032220E-008
9	7.9528314678 5241689019 4817612245 1032872937 5035650E-010
10	1.8774425910 0567756220 4988130993 7541387605 437996E-011
11	3.8247968264 1809029592 4653344686 7070280382 2264E-013
12	6.8432943010 1907998578 8027623030 3596055059 29E-015
13	1.0762104093 0537917245 5417733813 6774703889 3E-016
14	1.5124110216 1988369105 9052478125 978137640E -018
15	2.0715738792 9770436279 3713783632 7032961E-0 20
16	1.3846671521 9900108771 8574969994 14568E-022
17	5.3288541784 7605238410 1301497951 755E-024
18	3.5079551301 2368023505 6432045696 E-027
19	-5.9656175104 9257472195 3065263300 E-027
20	5.2969138512 2627670501 874181389E -028
21	-2.5226985875 2718441504 10473445E- 029
22	6.0209616883 8744484633 512535E-03 1
23	1.8543035351 4383646428 76522E-032
24	-3.0176817670 7158240262 6353E-033
25	1.8757233170 6238133052 809E-034
26	-6.7714760730 2256395698 9E-036
27	3.7182598930 255841378E -038
28	1.4954203444 742341364E -038
29	-1.2728642729 99664053E- 039
30	6.0377265821 589225E-04 1
31	-1.3644496192 99721E-042
32	-5.3539191733 757E-044
33	7.8650740191 78E-045
34	-4.7690907071 0E-046
35	1.6535692458 E-047
36	-2.3890246E-0 50
37	-4.2646358E-0 50

An alternate procedure would be to determine $z(\zeta)$ directly from this equation subject to the boundary condition $\lim_{\zeta \to 0} z(\zeta)/\zeta = 1$. This equation is an identity in the exact theory and not an extra condition.

From the theoretical point of view the most satisfactory proceedure would be to construct a sufficiently accurate representation of, say, the Helmholtz free energy A that would provide adequately accurate derivatives $(\frac{\partial A}{\partial V})_T = -P$, and $(\frac{\partial A}{\partial T})_V = -S$. Using (3.13), (3.15) (ignoring the constant), and integrating (3.16) we have for the Helmholtz free energy,

$$A = -P\Omega + (Z+1)NkT \log \zeta + ZNkT \log[z(\zeta)/\zeta]$$

$$= NkT \left[(Z+1)(\log \zeta - 1) + Z \int_0^\zeta [g(\eta) - 1]\frac{d\eta}{\eta} \right], \qquad (3.17)$$

for which the series expansion in ζ can be easily derived from Table 1. The inability to assign an absolute entropy for the ordinary ideal gas, leaves A uncertain by a

linear term in T. It remains to be seen which of the procedures outlined above are computationally most efficient.

4. COMPARISON OF IDEAL FERMI GAS TO THOMAS-FERMI THEORY

We now show the extent of agreement for aluminum between the ideal Fermi gas and the Thomas-Fermi theory. We use the computer program of D. A. Liberman[12] to compute the T-F numbers. We present the results in the figures as contours of percentage differences (electron properties only).

For the pressure, Figure 1 shows in temperature-density parameter space the 1%, 10%, and 30% contours, as one goes from the top curve of the figure to the bottom, respectively. The expected feature is that for high-temperature and/or low density the ideal gas is accurate. The 10% contour, for example, will serve as our "hot envelope," that is to say, the limit of the validity of the "hot curve" approximation. For low-temperature and high-density the ideal Fermi gas is again a good representation of the T-F theory because the electrons are being forced to the pressure-ionized, degenerate, free electron gas. Since as the density increases the kinetic energy per atom is forced by the Pauli principle to increase proportional to the density to the two-thirds power (relativistic corrections are ignored here) and the potential energy is expected to increase only as the one-third power of density, the free-electron-gas energy becomes dominate. This effect is begining to be evident in the behavior of the 30% contour. The ranges of temperature and density shown are those of interest for a great many applications. Thus the ideal Fermi gas well reproduces the T-F pressure over a substantial region.

Figure 1. Pressure contours.

Figure 2. Energy contours.

Figure 2 shows the results for the internal energy. Here we see only the 10% and 30% contours because the ideal Fermi gas does not represent the T-F energy as well as it does the pressure. This result is at least partly due to what, in effect, is an extra term present in the T-F energy and not in the T-F pressure. The bound electrons do not contribute to the pressure but do have a large effect on the energy, for the temperature and density both small. Since the free gas has no bound electrons, there is more difficulty in matching the T-F energy. However, there is again a "hot envelope."

We did one other study that was beyond our original intent. Our goal is really not to find an analytic representation of the T-F theory, but to obtain a fit to the T-F with the zero-temperature isotherm subtracted. Thus it is of interest to compare just such a result to the ideal gas with its zero-temperature isotherm subtracted. We expect an even better correspondence between these pressures, with exact agreement both at low-density/high-temperature and zero temperature. Figure 3 shows again the 1%, 10%, and 30% contours for pressure and indeed there is improvement over Figure 1 with the "hot envelope" now at lower temperatures. We do not show the contours that appear at low temperature as they are not of interest to us in this study. The odd vertical steps arise because really the two contours at that point loop back under themselves and come back to the lower curves due to the forced agreement at zero temperature. We did not put in these loops because we felt that was a misrepresentation of the high-temperature behavior.

The energy contours with zero-temperature isotherm subtracted are not presented because the results did not turn out as well as for the pressure. This result is again caused by the absence of the bound state energy in the free Fermi gas.

In general we see the "hot envelope" and reasonable agreement between the free

Figure 3. Pressure contours for the zero temperature isotherm subtracted.

Fermi gas and T-F theory for a large region of pressure. We understand the difference between the pressure and internal energy.

REFERENCES

1. L. H. Thomas, Proc. Cambridge Phil. Soc. **23**, 542 (1927); E. Fermi, Z. Physik **48**, 73 (1928).
2. P. A. M. Dirac, Proc. Cambridge Phil. Soc. **26**,376 (1930).
3. R. P. Feynman, N. Metropolis, and E. Teller Phys. Rev. **73**, 1561 (1949).
4. R. D. Cowan and J. Ashkin, Phys. Rev. **105**, 144 (1957).
5. G. A. Baker, Jr., Am. J. Phys. **27**, 29 (1959).
6. A. S. Eddington, "The Internal Constitution of Stars" (Dover, 1959, New York).
7. N. G. Van Kampen, in "Fundamental Problems in Statistical Mechanics" edited by E. G. D. Cohen (Wiley, 1968, New York) pg. 306.
8. K. Huang, "Statistical Mechanics" (Wiley, 1963, New York).
9. E. T. Copson, "An Introduction to the Theory of Functions of a Complex Variable" (Oxford Univ. Press, 1948, London).
10. G.A. Baker, Jr, "Essentials of Padé Approximants" (Academic, 1975, New York); G. A. Baker, Jr. and P. R. Graves-Morris, "Padé Approximants, Part I: Basic Theory and Part II: Extensions and Applications" part of the "Encyclopedia of Mathematics and its Applications, Vols. 13 & 14" (Cambridge Univ. Press, 1981, London).

11. P. S. Epstein, "Textbook of Thermodynamics" (Wiley, 1937, New York).
12. D. A. Liberman, private communication. This computer code is a straightforward programing of the T-F theory as presented in reference 3.